Methallyl alcohol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 5.67e-11 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 3.95e-01

Confidence level: 9.17e-01

Nearest Neighbors from the Training Set

Image not found
2-Methylbut-1-ene
Measured: 6.10e-11
Predicted: 5.84e-11

Image not found
alpha-Methylstyrene
Measured: 5.20e-11
Predicted: 9.42e-11

Image not found
2-Methylpent-1-ene
Measured: 6.30e-11
Predicted: 6.77e-11

Image not found
Isobutene
Measured: 5.14e-11
Predicted: 5.17e-11

Image not found
3-Methylbuta-1,2-diene
Measured: 5.69e-11
Predicted: 5.91e-11